A Local Support Operator Diffusion Discretization Scheme for Hexahedral Meshes

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Support Operator Method Properties

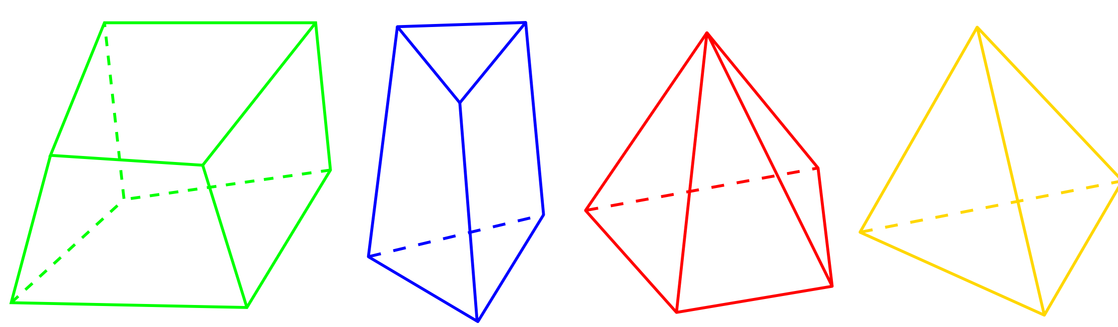
- It has a local stencil.
- It has both cell-centered and face-centered unknowns.
- It is conservative.
- Material discontinuities are treated rigorously.
- It generates a symmetric positive definite matrix.
- It is second-order accurate.
- It reduces to the standard differencing scheme if the mesh is orthogonal.
- It is not exact for linear functions.

Mesh Description

Multi-Dimensional Mesh:

Dimension	Geometries	Type of Elements
1-D	spherical, cylindrical or cartesian	line segments
2-D	cylindrical or cartesian	quadrilaterals or triangles
3-D	cartesian	hexahedra or degenerate hexahedra (tetrahedra, prisms, pyramids)

all with an unstructured (arbitrarily connected) format.



This presentation will assume a 3-D mesh.

Diffusion Equation Set

$$\alpha \frac{\partial \Phi}{\partial t} - \overrightarrow{\nabla} \cdot D \overrightarrow{\nabla} \Phi + \sigma \Phi = S$$

Which can be written

$$\alpha \frac{\partial \Phi}{\partial t} + \overrightarrow{\nabla} \cdot \overrightarrow{F} + \sigma \Phi = S$$

$$\overrightarrow{F} = -D \overrightarrow{\nabla} \Phi$$

Where

$$\begin{aligned} \Phi &= \text{Intensity} \\ \overrightarrow{F} &= \text{Flux} \\ D &= \text{Diffusion Coefficient} \\ \alpha &= \text{Time Derivative Coefficient} \\ \sigma &= \text{Removal Coefficient} \\ S &= \text{Intensity Source Term} \end{aligned}$$

Discretization Strategy

Cell-Center Equations – Integrate the Diffusion Equation over a cell, and temporally discretize via Backwards Euler:

$$\alpha^n \frac{\left(\Phi^{n+1} - \Phi^n\right)}{\Delta t} V_c + \sum_f \overrightarrow{F_{c,f}^{n+1}} \cdot \overrightarrow{A_{c,f}}$$

$$+ \sigma_c^n \Phi_c^{n+1} V_c = S_c^n V_c$$

Face Equations – Flux continuity at every face:

$$\overrightarrow{F_{c1,f1}^{n+1}} \cdot \overrightarrow{A_{c1,f1}} = -\overrightarrow{F_{c2,f2}^{n+1}} \cdot \overrightarrow{A_{c2,f2}}$$

Boundary Face Equations – Robin condition:

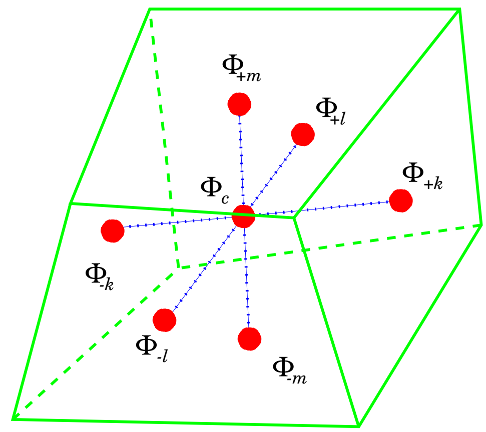
$$\beta_c^1 \Phi_{c,f} - \beta_c^2 \overrightarrow{F_{c,f}^{n+1}} \cdot \overrightarrow{A_{c,f}} = \beta_c^3 \Phi_b$$

Note that:

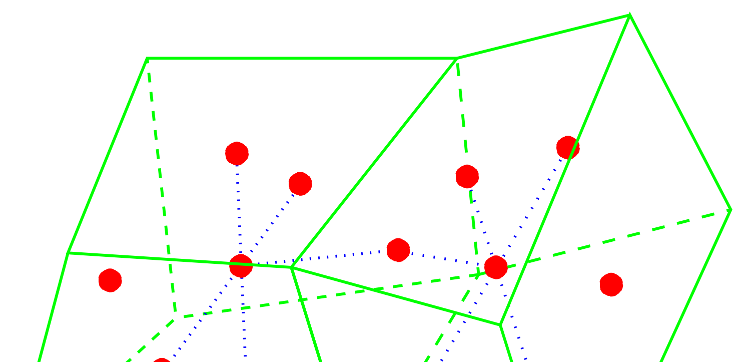
- This discretization will be inherently conservative.
- No derivatives are taken across material boundaries – a rigorous treatment.
- $\overrightarrow{F_{c,f}^{n+1}} \cdot \overrightarrow{A_{c,f}}$ remains to be defined (in terms of Φ).

Discretization Strategy

Unknowns for Φ are located at the cell centers and the cell faces. Cell Equations will involve these seven unknowns:



Face Equations will involve the thirteen unknowns from two adjacent cells:



This gives a local stencil in terms of cell-center and cell-face unknowns.

The $\overrightarrow{F_{c,f}^{n+1}} \cdot \overrightarrow{A_{c,f}}$ terms, on each face of a cell, must still be defined in terms of the Φ's within that cell.

Support Operator Method Derivation: Outline

The Support Operator Method for Diffusion on Hexahedra:

- Represent the diffusion term ($\overrightarrow{\nabla} \cdot D \overrightarrow{\nabla} \Phi$) as the divergence ($\overrightarrow{\nabla} \cdot$) of a gradient ($\overrightarrow{\nabla}$)

- Explicitly define one of the operators (in this case, the divergence operator)

- Define the remaining operator (in this case, the gradient operator) as the discrete adjoint of the first operator

- The previous step is accomplished by discretizing a portion of a vector identity

In other words, the first operator is set up explicitly, and the second operator is defined in terms of the first operator's definition.

Support Operator Method Derivation

Starting with a vector identity,

$$\overrightarrow{\nabla} \cdot \left(\phi \overrightarrow{W} \right) = \phi \overrightarrow{\nabla} \cdot \overrightarrow{W} + \overrightarrow{W} \cdot \overrightarrow{\nabla} \phi \, ,$$

where ϕ is the scalar variable to be diffused and $\overrightarrow{W}$ is an arbitrary vector, integrate over a cell volume:

$$\int_c \overrightarrow{\nabla} \cdot \left(\phi \overrightarrow{W} \right) dV = \int_c \phi \overrightarrow{\nabla} \cdot \overrightarrow{W} \, dV + \int_c \overrightarrow{W} \cdot \overrightarrow{\nabla} \phi \, dV \, .$$

Each colored term in the equation above will be treated separately.

Support Operator Method Derivation

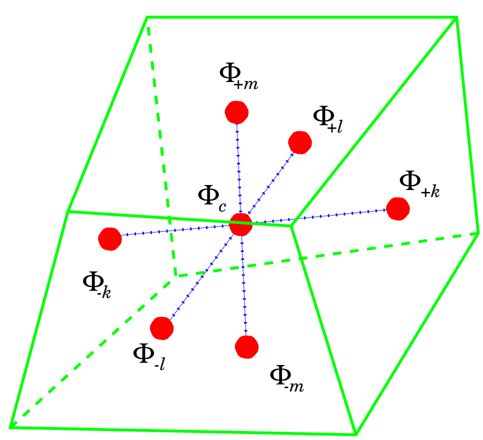
The Green term can be transformed via Gauss's Theorem into a surface integral,

$$\int_c \overrightarrow{\nabla} \cdot \left(\phi \overrightarrow{W}\right) \, dV = \oint_S \left(\phi \overrightarrow{W}\right) \cdot \overrightarrow{dA} \; .$$

This is discretized into values defined on each face of the hexahedral cell,

$$\oint_S \left(\phi \overrightarrow{W}\right) \cdot \overrightarrow{dA} \approx \sum_f \phi_f \overrightarrow{W_f} \cdot \overrightarrow{A_f} \; .$$

The summation over faces ($\sum_f$) includes six faces ($+\boldsymbol{k}$, $-\boldsymbol{k}$, $+\boldsymbol{l}$, $-\boldsymbol{l}$, $+\boldsymbol{m}$, $-\boldsymbol{m}$), shown here for the intensity variable ϕ:



Support Operator Method Derivation

The Red term is approximated by first assuming that ϕ is constant over the cell (at the center value), and then performing a discretization similar to the previous one for the Green term:

$$\begin{aligned}
\int_c \phi \, \overrightarrow{\nabla} \cdot \overrightarrow{W} \, dV &\approx \phi_c \int_c \overrightarrow{\nabla} \cdot \overrightarrow{W} \, dV \,, \\
&= \phi_c \oint_S \overrightarrow{W} \cdot \overrightarrow{dA} \,, \\
&\approx \phi_c \sum_f \overrightarrow{W_f} \cdot \overrightarrow{A_f} \,.
\end{aligned}$$

Support Operator Method Derivation

Turning to the final Blue term, insert the definition of the flux,

$$\overrightarrow{F} = -D\,\overrightarrow{\nabla}\,\phi\;,$$

to get

$$\int_c \overrightarrow{W} \cdot \overrightarrow{\nabla}\,\phi\,dV = -\int_c D^{-1}\,\overrightarrow{W} \cdot \overrightarrow{F}\,dV\;.$$

Note that by defining the flux in terms of the remainder of the equation, the gradient is being defined in terms of the divergence.

The Blue term is discretized by evaluating the integrand at each of the cell nodes (octants in 3-D) and summing:

$$-\int_c D^{-1}\,\overrightarrow{W} \cdot \overrightarrow{F}\,dV \approx -\sum_n D_n^{-1}\,\overrightarrow{W_n} \cdot \overrightarrow{F_n}\,V_n\;.$$

Support Operator Method Derivation

Combining all of the discretized terms of the colored equation and changing to a linear algebra representation gives

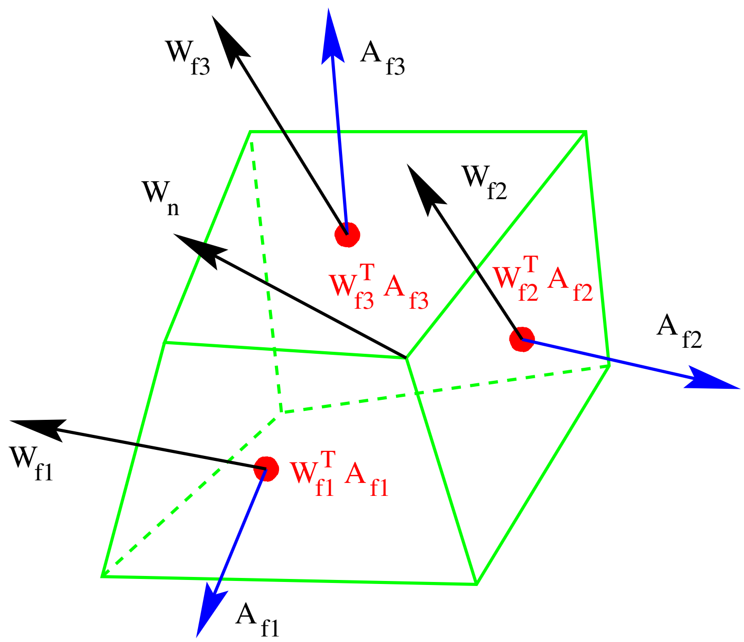
$$\sum_f \phi_f \mathbf{W}_f^{\mathrm{T}} \mathbf{A}_f = \phi_c \sum_f \mathbf{W}_f^{\mathrm{T}} \mathbf{A}_f - \sum_n D_n^{-1} \mathbf{W}_n^{\mathrm{T}} \mathbf{F}_n V_n \ .$$

Rearranging terms gives

$$\sum_n D_n^{-1} \mathbf{W}_n^{\mathrm{T}} \mathbf{F}_n V_n = \sum_f \left(\phi_c - \phi_f\right) \mathbf{W}_f^{\mathrm{T}} \mathbf{A}_f \ .$$

Note that the right hand side is a sum over the six faces, but the left hand side is a sum over the eight nodes.

Support Operator Method Derivation



In order to express the node-centered vectors, $\mathbf{W}_n$ and $\mathbf{F}_n$, in terms of their face-centered counterparts, define

$$\mathbf{J}_n^{\mathrm{T}}\mathbf{W}_n \equiv \begin{bmatrix} \mathbf{W}_{f1}^{\mathrm{T}}\mathbf{A}_{f1} \\ \mathbf{W}_{f2}^{\mathrm{T}}\mathbf{A}_{f2} \\ \mathbf{W}_{f3}^{\mathrm{T}}\mathbf{A}_{f3} \end{bmatrix},$$

where $f1$, $f2$, and $f3$ are the faces adjacent to node n and the Jacobian matrix is the square matrix given by

$$\mathbf{J}_n = \begin{bmatrix} \mathbf{A}_{f1} & \mathbf{A}_{f2} & \mathbf{A}_{f3} \end{bmatrix}.$$

Support Operator Method Derivation

Using this definition for the node-centered vectors $\mathbf{W}_n$ and $\mathbf{F}_n$ and performing some algebraic manipulations results in

$$\sum_n D_n^{-1} V_n \begin{bmatrix} \mathbf{W}_{f1}^{\mathrm{T}} \mathbf{A}_{f1} \\ \mathbf{W}_{f2}^{\mathrm{T}} \mathbf{A}_{f2} \\ \mathbf{W}_{f3}^{\mathrm{T}} \mathbf{A}_{f3} \end{bmatrix}^{\mathrm{T}} \mathbf{J}_n^{-1} \mathbf{J}_n^{-\mathrm{T}} \begin{bmatrix} \mathbf{F}_{f1}^{\mathrm{T}} \mathbf{A}_{f1} \\ \mathbf{F}_{f2}^{\mathrm{T}} \mathbf{A}_{f2} \\ \mathbf{F}_{f3}^{\mathrm{T}} \mathbf{A}_{f3} \end{bmatrix} = \widetilde{\mathbf{W}}^{\mathrm{T}} \tilde{\mathbf{\Phi}} \,.$$

where the sum over faces has been written as a dot product of $\widetilde{\mathbf{W}}$ and $\tilde{\mathbf{\Phi}}$, which are defined by

$$\widetilde{\mathbf{W}} = \begin{bmatrix} \mathbf{W}_1^{\mathrm{T}} \mathbf{A}_1 \\ \mathbf{W}_2^{\mathrm{T}} \mathbf{A}_2 \\ \mathbf{W}_3^{\mathrm{T}} \mathbf{A}_3 \\ \mathbf{W}_4^{\mathrm{T}} \mathbf{A}_4 \\ \mathbf{W}_5^{\mathrm{T}} \mathbf{A}_5 \\ \mathbf{W}_6^{\mathrm{T}} \mathbf{A}_6 \end{bmatrix} , \quad \tilde{\mathbf{\Phi}} = \begin{bmatrix} (\phi_c - \phi_1) \\ (\phi_c - \phi_2) \\ (\phi_c - \phi_3) \\ (\phi_c - \phi_4) \\ (\phi_c - \phi_5) \\ (\phi_c - \phi_6) \end{bmatrix} .$$

Support Operator Method Derivation

To convert the short vectors involving the faces adjacent to a particular node into sparse long vectors involving all of the faces of the cell, define permutation matrices for each node, $\mathbf{P}_n$, such that

$$\begin{bmatrix} \mathbf{W}_{f1}^{\mathrm{T}}\mathbf{A}_{f1} \\ \mathbf{W}_{f2}^{\mathrm{T}}\mathbf{A}_{f2} \\ \mathbf{W}_{f3}^{\mathrm{T}}\mathbf{A}_{f3} \end{bmatrix} = \mathbf{P}_n \begin{bmatrix} \mathbf{W}_1^{\mathrm{T}}\mathbf{A}_1 \\ \mathbf{W}_2^{\mathrm{T}}\mathbf{A}_2 \\ \mathbf{W}_3^{\mathrm{T}}\mathbf{A}_3 \\ \mathbf{W}_4^{\mathrm{T}}\mathbf{A}_4 \\ \mathbf{W}_5^{\mathrm{T}}\mathbf{A}_5 \\ \mathbf{W}_6^{\mathrm{T}}\mathbf{A}_6 \end{bmatrix} = \mathbf{P}_n \widetilde{\mathbf{W}} \ ,$$

where, for example,

$$\mathbf{P}_n = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{bmatrix} \qquad \begin{array}{l} \text{if } f1\,(n) = 3, \\ f2\,(n) = 5, \\ \text{and } f3\,(n) = 2. \end{array}$$

Note that $\mathbf{P}_n$ is rectangular, with a size of $N_d \times N_{lf}$ (3×6 for 3-D, 2×4 for 2-D, 1×2 for 1-D).

Support Operator Method Derivation

Using the permutation matrices, and defining $\widetilde{\mathbf{F}}$ in a fashion similar to $\widetilde{\mathbf{W}}$ ($\widetilde{\mathbf{F}}$ is a vector of $\mathbf{F}_f^{\mathrm{T}}\mathbf{A}_f$ for each cell face), gives

$$\sum_n D_n^{-1} V_n \widetilde{\mathbf{W}}^{\mathrm{T}} \mathbf{P}_n^{\mathrm{T}} \mathbf{J}_n^{-1} \mathbf{J}_n^{-\mathrm{T}} \mathbf{P}_n \widetilde{\mathbf{F}} = \widetilde{\mathbf{W}}^{\mathrm{T}} \widetilde{\mathbf{\Phi}} \ ,$$

or

$$\widetilde{\mathbf{W}}^{\mathrm{T}} \left[\sum_n D_n^{-1} V_n \mathbf{P}_n^{\mathrm{T}} \mathbf{J}_n^{-1} \mathbf{J}_n^{-\mathrm{T}} \mathbf{P}_n \right] \widetilde{\mathbf{F}} = \widetilde{\mathbf{W}}^{\mathrm{T}} \widetilde{\mathbf{\Phi}} \ ,$$

or

$$\widetilde{\mathbf{W}}^{\mathrm{T}} \mathbf{S} \widetilde{\mathbf{F}} = \widetilde{\mathbf{W}}^{\mathrm{T}} \widetilde{\mathbf{\Phi}} \ ,$$

where

$$\mathbf{S} = \sum_n D_n^{-1} V_n \mathbf{P}_n^{\mathrm{T}} \mathbf{J}_n^{-1} \mathbf{J}_n^{-\mathrm{T}} \mathbf{P}_n \ .$$

The original vector $\overrightarrow{W}$ (on which $\mathbf{W}_f$ and $\widetilde{\mathbf{W}}$ are based) was an arbitrary vector. It can now be eliminated from the equation to give

$$\mathbf{S} \widetilde{\mathbf{F}} = \widetilde{\mathbf{\Phi}} \ ,$$

which can easily be inverted to give the fluxes (dotted into the areas) in terms of the ϕ-differences, $\widetilde{\mathbf{F}} = \mathbf{S}^{-1} \widetilde{\mathbf{\Phi}}$. This is exactly the form needed for the discretization of the $\overrightarrow{F_{c,f}^{n+1}} \cdot \overrightarrow{A_{c,f}}$ term.

Support Operator Method Derivation: SPD Proof

The matrix $\mathbf{S}$ is symmetric, since

$$\begin{aligned}
\mathbf{S}^{\mathrm{T}} &= \left[\sum_n D_n^{-1} V_n \mathbf{P}_n^{\mathrm{T}} \mathbf{J}_n^{-1} \mathbf{J}_n^{-\mathrm{T}} \mathbf{P}_n\right]^{\mathrm{T}} \\
&= \sum_n D_n^{-1} V_n \left[\mathbf{P}_n^{\mathrm{T}} \mathbf{J}_n^{-1} \mathbf{J}_n^{-\mathrm{T}} \mathbf{P}_n\right]^{\mathrm{T}} \\
&= \sum_n D_n^{-1} V_n \left[\mathbf{J}_n^{-\mathrm{T}} \mathbf{P}_n\right]^{\mathrm{T}} \left[\mathbf{P}_n^{\mathrm{T}} \mathbf{J}_n^{-1}\right]^{\mathrm{T}} \\
&= \sum_n D_n^{-1} V_n \mathbf{P}_n{}^{\mathrm{T}} \mathbf{J}_n^{-1} \mathbf{J}_n^{-\mathrm{T}} \mathbf{P}_n \\
&= \mathbf{S}
\end{aligned}$$

The matrix $\mathbf{S}$ is positive definite, since

$$\begin{aligned}
\mathbf{x}^{\mathrm{T}} \mathbf{S} \mathbf{x} &= \sum_n D_n^{-1} V_n \mathbf{x}^{\mathrm{T}} \mathbf{P}_n^{\mathrm{T}} \mathbf{J}_n^{-1} \mathbf{J}_n^{-\mathrm{T}} \mathbf{P}_n \mathbf{x} \\
&= \sum_n D_n^{-1} V_n \left[\mathbf{J}_n^{-\mathrm{T}} \mathbf{P}_n \mathbf{x}\right]^{\mathrm{T}} \left[\mathbf{J}_n^{-\mathrm{T}} \mathbf{P}_n \mathbf{x}\right] \\
&= \sum_n D_n^{-1} V_n \left\| \mathbf{J}_n^{-\mathrm{T}} \mathbf{P}_n \mathbf{x} \right\|_2 \\
&> 0 \qquad \text{if } D_n^{-1} V_n > 0 \text{ and } \mathbf{J}_n^{-\mathrm{T}} \mathbf{P}_n \mathbf{x} \neq 0
\end{aligned}$$

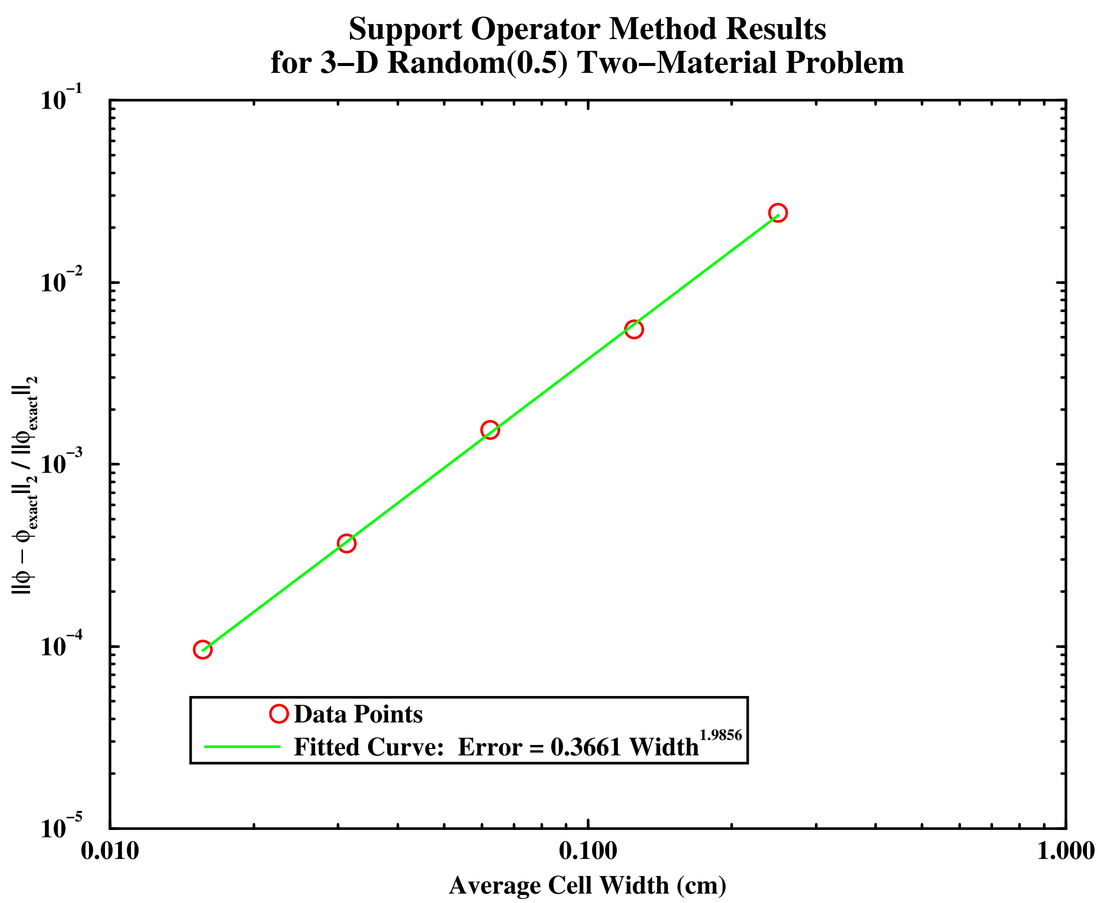
If $\mathbf{S}$ is SPD, then $\mathbf{S}^{-1}$ is also symmetric positive definite.

This is necessary, but not sufficient, to proving that the entire method is SPD. See the associated paper for the gory details.

Second-Order Demonstration

Two-material problem, ratio = 10, GMRES/CG, Low-Order Preconditioner, $\epsilon = 10^{-10}$, $\epsilon_{pre} = 10^{-9}$, SO

Problem Size (cells)	$\frac{\|\Phi_{\text{exact}} - \Phi\|_2}{\|\Phi_{\text{exact}}\|_2}$	Error Ratio
$2 \times 2 \times 2$	7.4950×10^{-2}	
$4 \times 4 \times 4$	2.4163×10^{-2}	3.10
$8 \times 8 \times 8$	5.5245×10^{-3}	4.37
$16 \times 16 \times 16$	1.5467×10^{-3}	3.57
$32 \times 32 \times 32$	3.6797×10^{-4}	4.20
$64 \times 64 \times 64$	9.6113×10^{-5}	3.82



Summary

- The Support Operator Methodology has been extended to 3-D Unstructured Hexahedral Meshes.
- It has a local stencil, with both cell-centered and face-centered unknowns.
- It is conservative and material discontinuities are treated rigorously.
- It generates a symmetric positive definite matrix.
- It is second-order accurate.
- It reduces to the standard differencing scheme if the mesh is orthogonal.

Diffusion Discretization References

1. J. E. Morel, Michael L. Hall, and Mikhail J. Shashkov. A Local Support-Operators Diffusion Discretization Scheme for Hexahedral Meshes. Submitted to *Journal of Computational Physics*, 1999. Available on-line at `http://www.lanl.gov/Caesar/`.

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3. Michael L. Hall and Jim E. Morel. A Second-Order Cell-Centered Diffusion Differencing Scheme for Unstructured Hexahedral Lagrangian Meshes. In *Proceedings of the 1996 Nuclear Explosives Code Developers Conference (NECDC), UCRL-MI-124790*, pages 359–375, San Diego, CA, October 21–25 1996. LA-CP-97-8. Available on-line at `http://www.lanl.gov/Caesar/`.

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